

(FILE 'HOME' ENTERED AT 16:59:40 ON 19 NOV 2005)

FILE 'REGISTRY' ENTERED AT 16:59:44 ON 19 NOV 2005

L1 1243 S MORPHINE
L2 3 S BUTAMBEN

FILE 'MEDLINE, BIOSIS, EMBASE, HCAPLUS' ENTERED AT 17:00:10 ON 19 NOV 2005

L3 33 S L1 AND L2
L4 30 DUP REM L3 (3 DUPLICATES REMOVED)

L4 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2005:244333 HCAPLUS

DN 143:307

TI Atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints: a promising approach for modeling of antibacterial activity

AU Marrero-Ponce, Yovani; Medina-Marrero, Ricardo; Torrens, Francisco; Martinez, Yamile; Romero-Zaldivar, Vicente; Castro, Eduardo A.

CS Department of Pharmacy, Faculty of Chemical-Pharmacy, Central University of Las Villas, Santa Clara, 54830, Cuba

SO Bioorganic & Medicinal Chemistry (2005), 13(8), 2881-2899

CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Ltd.

DT Journal

LA English

AB The Topol. Mol. Computer Design (TOMOCOMD-CARDD) approach has been introduced for the classification and design of antimicrobial agents using computer-aided mol. design. For this propose, atom, atom-type, and total quadratic indexes have been generalized to codify chemical structure information. In this sense, stochastic quadratic indexes have been introduced for the description of the mol. structure. These stochastic fingerprints are based on a simple model for the intramol. movement of all valence-bond electrons. In this work, a complete data set containing 1006 antimicrobial agents is collected and presented. Two structure-based antibacterial activity classification models have been generated. The models (including nonstochastic and stochastic indexes) classify correctly more than 90% of 1525 compds. in training sets. These models permit the correct classification of 92.28% and 89.31% of 505 compds. in an external test sets. The approach, also, satisfactorily compares with respect to nine of the most useful models for antimicrobial selection reported to date. Finally, a virtual screening of 87 new compds. reported in the anti-infective field with antibacterial activities is developed showing the ability of the models to identify new leads as antibacterial.

RE.CNT 91 THERE ARE 91 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2005:485667 HCAPLUS

DN 143:165983

TI Ligand-Based Virtual Screening and in Silico Design of New Antimalarial Compounds Using Nonstochastic and Stochastic Total and Atom-Type Quadratic Maps

AU Marrero-Ponce, Yovani; Iyarreta-Veitia, Maite; Montero-Torres, Alina; Romero-Zaldivar, Carlos; Brandt, Carlos A.; Avila, Priscilla E.; Kirchgatter, Karin; Machado, Yanetsy

CS Department of Pharmacy, Faculty of Chemical Pharmacy and Department of Drug Design, Chemical Bioactive Center, Central University of Las Villas, Santa Clara, Villa Clara, 54830, Cuba

SO Journal of Chemical Information and Modeling (2005), 45(4), 1082-1100

CODEN: JCISD8; ISSN: 1549-9596

PB American Chemical Society

DT Journal

LA English

AB Malaria has been one of the most significant public health problems for centuries. It affects many tropical and subtropical regions of the world. The increasing resistance of Plasmodium spp. to existing therapies has heightened alarms about malaria in the international health community. Nowadays, there is a pressing need for identifying and developing new drug-based antimalarial therapies. In an effort to overcome this problem, the main purpose of this study is to develop simple linear discriminant-based quant. structure-activity relation (QSAR) models for the classification and prediction of antimalarial activity using some of the TOMOCOMD-CARDD (Topol. Mol. COMputer Design-Computer Aided "Rational" Drug Design) fingerprints, to enable computational screening from virtual combinatorial datasets. In this sense, a database of 1562 organic chems. having great structural variability, 597 of them antimalarial agents and 965 compds. having other clin. uses, was analyzed and presented as a helpful tool, not only for theor. chemists but also for other researchers

in this area. This series of compds. was processed by a k-means cluster anal. to design training and predicting sets. Afterward, two linear classification functions were derived to discriminate between antimalarial and nonantimalarial compds. The models (including nonstochastic and stochastic indexes) correctly classify more than 93% of the compound set, in both training and external prediction datasets. They showed high Matthews' correlation coeffs., 0.889 and 0.866 for the training set and 0.855 and 0.857 for the test one. The models' predictivity was also assessed and validated by the random removal of 10% of the compds. to form a new test set, for which predictions were made using the models. The overall means of the correct classification for this process (leave group 10% full-out cross validation) using the equations with nonstochastic and stochastic atom-based quadratic fingerprints were 93.93% and 92.77%, resp. The quadratic maps-based TOMOCOMD-CARDD approach implemented in this work was successfully compared with four of the most useful models for antimalarials selection reported to date. The developed models were then used in a simulation of a virtual search for Ras FTase (FTase = farnesyltransferase) inhibitors with antimalarial activity; 70% and 100% of the 10 inhibitors used in this virtual search were correctly classified, showing the ability of the models to identify new lead antimalarials. Finally, these two QSAR models were used in the identification of previously unknown antimalarials. In this sense, three synthetic intermediaries of quinolinic compds. were evaluated as active/inactive ones using the developed models. The synthesis and biol. evaluation of these chems. against two malaria strains, using chloroquine as a reference, was performed. An accuracy of 100% with the theor. predictions was observed. Compound 3 showed antimalarial activity, being the first report of an arylaminomethylenemalonate having such behavior. This result opens a door to a virtual study considering a higher variability of the structural core already evaluated, as well as of other chems. not included in this study. We conclude that the approach described here seems to be a promising QSAR tool for the mol. discovery of novel classes of antimalarial drugs, which may meet the dual challenges posed by drug-resistant parasites and the rapid progression of malaria illnesses.

RE.CNT 111 THERE ARE 111 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:753122 HCAPLUS
DN 141:266040
TI Joint prosthesis with polymer matrix for sustained release of a
therapeutic agent
IN Tunc, Deger C.; Ranawat, Chitranjan S.; Ranawat, Almar S.; Banks, James
Ronald
PA Howmedica Osteonics Corp., USA
SO Eur. Pat. Appl., 38 pp.
CODEN: EPXXDW

DT Patent
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1457172	A1	20040915	EP 2004-251143	20040227
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK, HR				
	US 2004180072	A1	20040916	US 2003-387315	20030312
	CA 2458761	AA	20040912	CA 2004-2458761	20040223
	JP 2004277421	A2	20041007	JP 2004-70199	20040312
PRAI	US 2003-387315	A	20030312		

AB A device for releasing a therapeutic agent in the body space in the form of a prosthetic joint implant having a first portion such as a stemmed portion for contacting bone tissue in an intramedullary canal of a long bone is described. The implant has a second portion which extends into the body space such as a joint space. The joint component contains a reservoir filled with a bioabsorbable/resorbable polymer which includes a therapeutic agent. The reservoir is open or in contact with the joint space as the body fluid diffuses in and out of the polymeric device it carries the drug into the joint space. For example, 120 g of polymer,

poly(DL-lactide/glycolide), 50:50 mol ratio, was dry blended with 180 g of bupivacaine and melt blended. The extrudate was ground to a particle size of 3 to 5 mm, melted and extruded into rods of diameter of 7.87 mm. A cylinder having a length of 21.3 mm was cut. The rod had a surface area of 622.9 mm², weighed 1.20 g, and had 60% drug by weight. The cylindrical rod was coated with a 5% solution of poly(DL-lactide/glycolide), 50:50 ratio, in dioxane and vacuum dried. The rate of drug release can be controlled by changing the level of drug loading in the device.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 30 MEDLINE on STN DUPLICATE 1
AN 2003439311 MEDLINE
DN PubMed ID: 14500165
TI Analgesic synergy between topical morphine and butamben in mice.
AU Kolesnikov Yuri A; Cristea Marcela; Pasternak Gavril W
CS Department of Anesthesiology, Memorial-Sloan Kettering Cancer Center, New York, New York 10021, USA.. kolesniy@mskcc.org
NC DA00220 (NIDA)
DA00405 (NIDA)
DA07241 (NIDA)
SO Anesthesia and analgesia, (2003 Oct) 97 (4) 1103-7, table of contents.
Journal code: 1310650. ISSN: 0003-2999.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
LA English
FS Abridged Index Medicus Journals; Priority Journals
EM 200310
ED Entered STN: 20030923
Last Updated on STN: 20031015
Entered Medline: 20031014
AB Studies have revealed that lidocaine is an effective analgesic when applied topically to the tail of a mouse in the radiant heat tail-flick assay. In addition, the topical combination of lidocaine with morphine revealed synergistic interactions between the two drugs. In the current studies, we demonstrate that topical butamben, benzocaine, and bupivacaine are active in the radiant heat tail-flick assay. In this assay, topical lidocaine has a ceiling effect and displays a biphasic curve, with large doses markedly decreasing the responses almost to baseline levels. In contrast, butamben has an S-shape dose-dependent response in the assay and did not display a biphasic curve as seen with lidocaine, suggesting that topical butamben may have advantages over lidocaine. Both benzocaine and bupivacaine also showed dose-dependent analgesic activity in this model. Like lidocaine, butamben/morphine combinations displayed synergistic interactions. Indeed, the synergy appeared more prominent with a butamben/morphine combination. We also observed synergy between topical benzocaine and morphine. Although the bupivacaine/morphine combination was suggestive of synergy on isobolographic analysis, it did not achieve statistical significance. These studies indicate that a series of local anesthetics are all active topically in the radiant heat tail-flick assay in mice and that several interact synergistically with morphine. Of the local anesthetics tested, butamben seemed to have several pharmacological characteristics, alone and in combination with morphine, which suggest that it may be superior to the other local anesthetics. Together, these observations suggest that topical combinations of opioids and local anesthetics may prove clinically valuable. IMPLICATIONS: Topical administration of the opioid micro-agonist morphine and the sodium channel inhibitors butamben and benzocaine results in a synergistic interaction for antinociception in radiant heat tail-flick assay in mice, suggesting that the combination of these drugs will enhance rather than detract from the analgesia of either alone.

L4 ANSWER 5 OF 30 EMBASE COPYRIGHT (c) 2005 Elsevier B.V. All rights reserved on STN
AN 2003343371 EMBASE
TI EUS-guided celiac plexus neurolysis - Technique and indication.
AU Schmulewitz N.; Hawes R.
CS Dr. R. Hawes, Digestive Disease Center, Medical University of South

Carolina, 171 Ashley Avenue, Charleston, SC 29425-2220, United States.
 HawesR@muscc.edu
 SO Endoscopy, (1 Aug 2003) Vol. 35, No. 8, pp. S49-S53.
 Refs: 56
 ISSN: 0013-726X CODEN: ENDCAM
 CY Germany
 DT Journal; Conference Article
 FS 008 Neurology and Neurosurgery
 027 Biophysics, Bioengineering and Medical Instrumentation
 048 Gastroenterology
 014 Radiology
 037 Drug Literature Index
 030 Pharmacology
 016 Cancer
 038 Adverse Reactions Titles
 036 Health Policy, Economics and Management
 LA English
 ED Entered STN: 20041018
 Last Updated on STN: 20041018
 DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

L4 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:589718 HCAPLUS
 DN 138:260224
 TI Prediction of aqueous solubility of organic compounds using a quantitative
 structure-property relationship
 AU Chen, Xue-Qing; Cho, Sung Jin; Li, Yi; Venkatesh, Srini
 CS L12-09, Preclinical Candidate Optimization, Bristol-Myers Squibb
 Pharmaceutical Research Institute, Discovery Pharmaceuticals, Lawrenceville,
 NJ, 08543, USA
 SO Journal of Pharmaceutical Sciences (2002), 91(8), 1838-1852
 CODEN: JPMSAE; ISSN: 0022-3549
 PB Wiley-Liss, Inc.
 DT Journal
 LA English
 AB A quant. structure-property relationship (QSPR) was developed for
 predicting the aqueous solubility of drug-like compds. from their chemical structures.
 A set of 321 structurally diverse drugs or related compds., with their
 intrinsic aqueous solubility collected from literature, was used in this anal. The
 data were divided into a training set (n = 267) for building the model and
 a randomly chosen testing set (n = 54) for assessing the predictive
 ability of the model. A series of mol. descriptors was calculated directly
 from chemical structures and a set of eight descriptors, including dipole
 moment, surface area, volume, mol. weight, number of rotatable bonds/total bonds,
 number of hydrogen-bond acceptors, number of hydrogen-bond donors and d., was
 chosen for the final model. The eight-descriptor model generated by
 multiple linear regression was further optimized by a genetic algorithm
 guided selection method. The model has a correlation coefficient (r) of 0.95
 and a root-mean-square (rms) error of 0.56 log unit. It predicts the
 solubility of testing set compds. with a reasonable degree of accuracy (r =
 0.84 and rms = 0.86 log unit). The present model can serve as a tool for
 medicinal chemists to guide their early synthetic efforts in arriving at
 appropriate analogs.

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:612596 HCAPLUS
 DN 138:343605
 TI Study of crystalline drugs by means of a polarizing microscope. XIX. A
 trial production of a table of the optical crystallographic
 characteristics of crystalline drugs including crystal habits
 AU Watanabe, Atsushi
 CS Kenbikogaku-Kenkyusho Ltd., 7-4, Matsunouchi-cho, Ashiya City, 659-0094,
 Japan
 SO Yakugaku Zasshi (2002), 122(8), 595-606
 CODEN: YKKZAJ; ISSN: 0031-6903
 PB Pharmaceutical Society of Japan

DT Journal
 LA Japanese
 AB It was clarified in previous report that the predominant faces of crystal habits mainly coincide with the morphol. crystal face at (001), (010), or (100), and therefore the two measurable key refractive indexes are closely related to the principal sections of the two axial wave surfaces and coincide with the one or two of the three principal refractive indexes. The three principal refractive indexes of biaxial crystalline drugs were measured and tabulated in the "General Information" section of the National Formulary compiled by the American Pharmaceutical Association. A series of studies was conducted to measure the key refractive indexes of the crystalline drugs listed in the Japanese Pharmacopoeia X or XI so that the data could be used to improve the quant. anal. of their crystal habits. The purpose of the present study was to examine data on both the key and principal refractive indexes and attempt to produce a general authorized table of optic crystallog. characteristics, including crystal habits, for simpler and more reliable polarizing microscopy studies.

L4 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2000:553397 HCAPLUS
 DN 133:168375
 TI Method of manufacture for transdermal matrixes
 IN Audett, Jay D.; Detroyer, Georges D.
 PA Ortho-McNeil Pharmaceutical, Inc., USA
 SO PCT Int. Appl., 38 pp.
 CODEN: PIXXD2

DT Patent
 LA English
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000045797	A1	20000810	WO 2000-US2491	20000201
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 1999-241662	A	19990202		

AB Disclosed is a method of manufacture for the production of transdermal drug delivery matrixes and devices, transdermal sampling devices, and dermal conditioning devices. A polymer and an active agent are mixed and heated in a multiple-lobed compounder to produce a polymer mixture. The polymer mixture is extruded and then at least a portion of the extrudate is formed into, for example, the transdermal drug delivery matrix, or incorporated into the transdermal drug delivery device. These alternative methods for preparing transdermal matrixes have several advantages over the current methods of manufacture. The matrix components, particularly the active agent, are not exposed to extremes in solvent or temperature for extended periods of time during the manufacture process. The transdermal matrixes prepared by these methods perform better in transdermal devices and show greater flux of active agent. As a result of the improved performance, less active agent may be utilized during the manufacturing process, and smaller or thinner transdermal matrixes may be produced for incorporation into the corresponding transdermal device. An olanzapine transdermal matrix was prepared using a twin screw extruder as follows; HMW polyisobutylene (Vistanex L80) was blended with LMW polyisobutylene, silica gel powder, and PVP. Sep., olanzapine and lauryl lactate were processed and blended with the polymeric mixts. The resulting mixture was extruded through a sheet die and coated between a release liner and backing material. A second layer of the same extrudate was coated between a second release liner and a polyester nonwoven porous supporting layer. The release liner from the first coating pass was removed and the exposed extrudate was laminated to the nonwoven side of the second coating pass, sandwiching the porous supporting layer between the two extrudates. The rolls of laminate were converted to transdermal devices of the desired size.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 30 EMBASE COPYRIGHT (c) 2005 Elsevier B.V. All rights reserved on STN
AN 2000394154 EMBASE
TI Novel drugs for neuropathic pain.
AU Kopf A.; Ruf W.
CS Dr. A. Kopf, Pain Management Centre, Dept. of Anaesthesiol./Intensive Care, Benjamin Franklin Univ. Hospital, Hindenburgdamm 30, 12200 Berlin, Germany. Kopf@ukbf.fu-berlin.de
SO Current Opinion in Anaesthesiology, (2000) Vol. 13, No. 5, pp. 577-583.
Refs: 72
ISSN: 0952-7907 CODEN: COAEE2
CY United Kingdom
DT Journal; General Review
FS 008 Neurology and Neurosurgery
024 Anesthesiology
037 Drug Literature Index
038 Adverse Reactions Titles
LA English
SL English
ED Entered STN: 20001213
Last Updated on STN: 20001213
AB Neuropathic pain is often inadequately controlled by conventional analgesics. Because the aetiology of neuropathic pain is only partially understood, specific treatment approaches have not been defined. A variety of pharmacological treatments have been proposed. However, for only a small minority of drugs used in neuropathic pain has the scientific evidence been evaluated in a satisfactory manner. The present review of the recent literature reveals the potential of certain novel drugs in treatment of neuropathic pain. (C) 2000 Lippincott Williams and Wilkins.

L4 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:510847 HCAPLUS
DN 131:314140
TI The correlation and prediction of the solubility of compounds in water using an amended solvation energy relationship
AU Abraham, Michael H.; Le, Joelle
CS Department of Chemistry, University College London, London, WC1H 0AJ, UK
SO Journal of Pharmaceutical Sciences (1999), 88(9), 868-880
CODEN: JPMSAE; ISSN: 0022-3549
PB American Chemical Society
DT Journal
LA English
AB The aqueous solubility of liqs. and solids, as log SW, has been correlated with an amended solvation equation that incorporates a term in $\Sigma\alpha_2H$ + $\Sigma\beta_2H$, where the latter are the hydrogen bond acidity and basicity of the solutes, resp. Application to a training set of 594 compds. led to a correlation equation with a standard deviation, SD, of 0.56 log units. For a test set of 65 compds., the SD was 0.50 log units, and for a combined correlation equation for 659 compds., the SD was 0.56 log units. The correlation equations enable the factors that influence aqueous solubility to be revealed. The hydrogen-bond propensity of a compound always leads to an increase in solubility, even though the $\Sigma\alpha_2H$ + $\Sigma\beta_2H$ term opposes solubility due to interactions in the liquid or solid. Increase in solute dipolarity/polarizability increases solubility, whereas an increase in solute excess molar refraction, and especially, volume decrease solubility. The solubility of Bronsted acids and bases is discussed, and corrections for the fraction of neutral species in the saturated solution are graphically presented.

RE.CNT 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 30 EMBASE COPYRIGHT (c) 2005 Elsevier B.V. All rights reserved on STN
AN 1999176316 EMBASE
TI Neuropathic pain: A GP's guide.

AU Brooker C.; Cousins M.J.; Molloy A.R.
 CS Dr. C. Brooker, Sydney's Univ. Pain Mgmt./Res. Ctr., Royal North Shore
 Hospital, Sydney, NSW, Australia
 SO Modern Medicine of Australia, (1999) Vol. 42, No. 5, pp. 58-68.
 Refs: 16
 ISSN: 1030-3782 CODEN: MMAUB7
 CY Australia
 DT Journal; General Review
 FS 008 Neurology and Neurosurgery
 037 Drug Literature Index
 LA English
 SL English
 ED Entered STN: 19990603
 Last Updated on STN: 19990603
 AB Neuropathic pain is a significant acute and chronic symptom of many
 diseases that is caused by a lesion or dysfunction in the nervous system.
 Early intervention is essential for patients with this type of pain.
 General practitioners have an important role in diagnosing and treating
 patients with neuropathic pain, and in referring patients to the
 appropriate specialists where necessary.

L4 ANSWER 12 OF 30 EMBASE COPYRIGHT (c) 2005 Elsevier B.V. All rights
 reserved on STN
 AN 1998279831 EMBASE
 TI The hydrophobic effect. 3. A key ingredient in predicting n-octanol- water
 partition coefficients.
 AU Ruelle P.; Kesselring U.W.
 CS P. Ruelle, Institut d'Analyse Pharmaceutique, Section de Pharmacie,
 Universite de Lausanne, CH-1015 Lausanne, Switzerland.
 Paul.Ruelle@iap.unil.ch
 SO Journal of Pharmaceutical Sciences, (1998) Vol. 87, No. 8, pp. 1015-1024.
 Refs: 53
 ISSN: 0022-3549 CODEN: JPMSAE
 CY United States
 DT Journal; Article
 FS 037 Drug Literature Index
 039 Pharmacy
 LA English
 SL English
 ED Entered STN: 19980917
 Last Updated on STN: 19980917
 AB The quantitative development of the mobile order theory in H-bonded
 liquids is extended to predict the n-octanol/water partition coefficient
 (P). The log P predictive equation strictly issued from a thermodynamic
 treatment reduces to a simple linear volume-log P relationship whose
 intercept and slope encode, respectively, the solvation and entropy
 effects. For noncomplexing substances, the partition coefficient values
 result from two volume-dependent entropic contributions reflecting (a) the
 difference in the exchange entropy between the solute and solvent
 molecules in the n-octanol and water phases, and (b) the propensity
 difference between the two H-bonded solvents to induce a hydrophobic
 effect toward the solute. Although both effects increase, although with
 opposite signs, compared with the growing molar volume of the partitioned
 compound, the hydrophobic contribution always predominates favoring the
 transfer of the solute into the organic phase and hence increasing its
 partition coefficient. When dealing with complexing chemicals, the
 hydrophobic effect-related term, though remaining the dominant factor in
 most cases, is more or less counterbalanced by the formation of H- bonds
 between the interacting sites of the solute and the n-octanol and water
 solvent molecules. The log P, corrected for the substantial content of
 water into n-octanol, is estimated for a number of compounds of
 environmental and pharmaceutical interest. The extent to which the
 entropic and enthalpic factors affect the overall partition coefficient
 value is analyzed.

L4 ANSWER 13 OF 30 EMBASE COPYRIGHT (c) 2005 Elsevier B.V. All rights
 reserved on STN
 AN 1998373861 EMBASE

TI Peripheral nerve blockade in the treatment of pain.
AU Fischer H.B.J.
CS H.B.J. Fischer, Alexandra Hospital NHS Trust, Woodrow Drive, Redditch,
Worcestershire B98 7UB, United Kingdom
SO Pain Reviews, (1998) Vol. 5, No. 3, pp. 183-202.
Refs: 108
ISSN: 0968-1302 CODEN: PAREFV
CY United Kingdom
DT Journal; General Review
FS 008 Neurology and Neurosurgery
024 Anesthesiology
037 Drug Literature Index
038 Adverse Reactions Titles
LA English
SL English
ED Entered STN: 19990115
Last Updated on STN: 19990115
AB Local anaesthetic blockade of the peripheral nervous system was
historically important in the provision of surgical anaesthesia and
postoperative analgesia. With increasing awareness of the potential
benefits of regional anaesthesia, there has been a resurgence of interest
in the role of peripheral nerve blockade in the management of pain.
Surgical anaesthesia remains the prime indication for major nerve blocks,
but they are now used more frequently to manage both acute and chronic
pain. There are no large prospective trials comparing peripheral nerve
blocks with either central neural blockade or general anaesthesia in terms
of improved outcome, but developments in peripheral multimodal analgesia,
new local anaesthetics and adjuvant drugs offer the potential for greater
patient benefit from peripheral nerve blocks in the future.

L4 ANSWER 14 OF 30 EMBASE COPYRIGHT (c) 2005 Elsevier B.V. All rights
reserved on STN

AN 1998081363 EMBASE
TI Pain management in a patient with medication allergies.
AU Simmonds M.A.; Du Pen S.L.; Ferrell B.R.
SO Cancer Practice, (1998) Vol. 6, No. 1, pp. 8-10.
ISSN: 1065-4704 CODEN: CAPRFJ

CY United States
DT Journal; Article
FS 014 Radiology
016 Cancer
030 Pharmacology
037 Drug Literature Index
038 Adverse Reactions Titles

LA English
ED Entered STN: 19980402
Last Updated on STN: 19980402
DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

L4 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:358925 HCAPLUS
DN 126:334422

TI Pharmaceutical emulsions containing a local anesthetic and/or centrally
acting analgesic
IN Toledo, Alfonso
PA B. Braun Melsungen Ag, Germany
SO Eur. Pat. Appl., 14 pp.
CODEN: EPXXDW

DT Patent
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 770387	A1	19970502	EP 1995-117034	19951028
	EP 770387	B1	19990811		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	AT 183092	E	19990815	AT 1995-117034	19951028
	ES 2138130	T3	20000101	ES 1995-117034	19951028

PRAI EP 1995-117034 A 19951028

AB A pharmaceutical composition in the form of an oil-in-water emulsion (o/w) consisting essentially of (a) 5 to 30% (w/v) of an oily carrier consisting of long-chain triglycerides and/or medium-chain triglycerides, (b) 0.5 to 2% (w/v) of an emulsifier, (c) 0.1 to 2% (w/v) of a local anesthetic and/or centrally acting analgesic, (d) conventional additives. An injectable submicron emulsion contained soya bean oil 10, miglyol 10, egg yolk lecithin 1.2, glycerol 2.5, sodium oleate 0.03, bupivacaine base (I) 0.4439 g, and water q.s. 100 mL. The amount of I encapsulated into the oil droplets was 99.0-99.8%. The emulsion significantly increased the duration of total motor blockade from 140.6 to 220.0 min and the recovery period from 218.3 to 303.1 min, when compared to the aqueous solution

L4 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:3273 HCAPLUS

DN 126:42183

TI Systematic analysis of basic drugs in plasma using X-5 solid-phase extraction GC-FID and GC-MS

AU Qiu, Fenghe; Liu, Li; Luo, Li; Liu, Feng; Lu, Yongquan

CS Institute Pharmacology Toxicology, Academy Military Medical Sciences, Beijing, 100850, Peop. Rep. China

SO Yaoxue Xuebao (1996), 31(4), 296-299

CODEN: YHHPAL; ISSN: 0513-4870

PB Chinese Academy of Medical Sciences, Institute of Materia Media

DT Journal

LA Chinese

AB A systematic determination method for 34 basic drugs in human plasma was developed. Thirty-four basic drugs such as diazepam and caffeine were extracted from plasma at pH 10 using X-5 resin as adsorbent, and then identified and quantified by capillary GC-FID and GC-MS. The detection limits for most drugs were in the range of 0.5-0.2 µg mL⁻¹, recovery was 79-103% and RSD was 1.1-11.5%.

L4 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:729623 HCAPLUS

DN 123:190633

TI Capillary zone electrophoresis in a comprehensive screen for basic drugs in whole blood

AU Hudson, J.C.; Golin, M.; Malcolm, M.

CS Toxicology Section, RCMP Forensic Laboratory, Regina, SK, S4P 3J7, Can.

SO Journal - Canadian Society of Forensic Science (1995), 28(2), 137-52

CODEN: JCFSBP; ISSN: 0008-5030

PB Canadian Society of Forensic Science

DT Journal

LA English

AB Capillary zone electrophoresis (CZE) is shown to be capable of detecting a large number of basic drugs at concns. considered to be forensically significant. A procedure for preparing exts. of whole blood for anal. by CZE is presented. Relative migration times are presented for over 400 drugs, analyzed using 100 mmol/L phosphate run buffer of pH 2.5 and pH 9.5.

L4 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:491751 HCAPLUS

DN 121:91751

TI Drug binding by reservoirs in elastomeric infusion devices

AU Jenke, Dennis R.

CS William B. Graham Science Center, Baxter Healthcare Corporation, Round Lake, IL, 60073, USA

SO Pharmaceutical Research (1994), 11(7), 984-9

CODEN: PHREEB; ISSN: 0724-8741

DT Journal

LA English

AB Drug binding by an elastomeric infusion device reservoir was assessed by measuring its ability to bind fifteen model solutes. Octanol/water and hexane/water partition coeffs. were regressed against the reservoir's solute equilibrium binding constant to generate a binding model. The reservoir's drug binding ability was calculated with the model and drug partition coeffs., which were determined for 17 commonly infused drugs including tobramycin,

gentamicin, penicillin G, piperacillin, lidocaine, morphine, ceftriaxone, imipenem-cilastatin, amphotericin B, ticarcillin and clavulanate, pentamidine, vancomycin, foscarnet, desferoxamine, acyclovir, fluconazole and vinblastine. Formulations studied included 0.9% saline and 5% Dextrose. With the exception of lidocaine, imipenem, vinblastine and fluconazole, octanol/ formulation and hexane/formulation partition coeffs. were too low to be measured for these drugs. Thus, the majority of the drugs, when reconstituted in 0.9% saline or 5% dextrose, will not be bound by the reservoirs. The magnitude of drug loss for the most highly bound species, fluconazole, is <2%. Therefore, the reservoirs used in this study are essentially inert with respect to binding of the drugs evaluated in this study.

L4 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:639786 HCAPLUS

DN 115:239786

TI An aqueous suspension containing a local anesthetic or analgesic for injections

IN Ackerman, Eric Willem; Grouls, Rene Jacobus Elisabeth; Korsten, Hendrikus Hubertus Maria

PA Stichting, Catharina Ziekenhuis, Neth.

SO PCT Int. Appl., 15 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9114455	A1	19911003	WO 1991-NL42	19910320
	W: AU, CA, FI, JP, NO, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
	NL 9000634	A	19911016	NL 1990-634	19900320
	CA 2077641	AA	19910921	CA 1991-2077641	19910320
	CA 2077641	C	20010703		
	AU 9175580	A1	19911021	AU 1991-75580	19910320
	AU 646857	B2	19940310		
	EP 521070	A1	19930107	EP 1991-906827	19910320
	EP 521070	B1	19950426		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 05507466	T2	19931028	JP 1991-507032	19910320
	AT 121631	E	19950515	AT 1991-906827	19910320
	ES 2074269	T3	19950901	ES 1991-906827	19910320
	NO 9203429	A	19920917	NO 1992-3429	19920903
	NO 300114	B1	19970414		
	FI 9204019	A	19920908	FI 1992-4019	19920908
	FI 98890	B	19970530		
	FI 98890	C	19970910		
	US 5346903	A	19940913	US 1992-979128	19921120
PRAI	NL 1990-634	A	19900320		
	WO 1991-NL42	A	19910320		

AB An injection solution comprises a water-insol. local anesthetic and/or narcotic analgesic in the form of particles suspended in an aqueous medium for epidural and intrathecal pain relief. The particles of the active agent have a mean diameter of <20 µm and >99% of the particles have a diameter of <100 µm. The preparation is stabilized by the addition of nonionic surface-active agent in an amount <1%. A sterile aqueous suspension containing Bu p-aminobenzoate 10, NaCl 0.9, and polysorbate 0.025% was prepared by the freeze-defrost technique. The suspension was administered epidurally to patients suffering from intractable pain due to cancer and long-lasting sensory blockade after repeated injections occurred.

L4 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1992:400277 HCAPLUS

DN 117:277

TI Mechanism of allergic cross-reactions. I. Multispecific binding of ligands to a mouse monoclonal anti-DNP IgE antibody

AU Varga, Janos M.; Kalchschmid, Gertrud; Klein, Georg F.; Fritsch, Peter

CS Dep. Dermatol., Univ. Innsbruck, Innsbruck, 6020, Austria

SO Molecular Immunology (1991), 28(6), 641-54
CODEN: MOIMD5; ISSN: 0161-5890

DT Journal

LA English

AB A recently developed solid-phase binding assay was used to investigate the specificity of ligand binding to a mouse monoclonal anti-dinitrophenyl IgE (I). All DNP-amino acids, that were tested inhibited the binding of the radio-labeled I to DNP covalently attached to polystyrene microplates; however, the concentration for 50% inhibition varied within four orders of magnitude, DNP-L-serine being the most and DNP-L-proline the least potent inhibitor. In addition to DNP analogs, a large number of drugs and other compds. were tested for their ability to compete with DNP for the binding site of I. At the concentration used for screening, 59% of compds. had no significant inhibition; 19% inhibited the binding of I more than 50%. Several families of compds. (tetracyclines, polymyxins, phenothiazines, salicylates, and quinones) that were effective competitors were found. Within these families, changes in the functional groups attached to the family stem had major effects on the affinity of ligand binding. The occurrence frequencies of interactions of ligands with I is in good agreement with the semi-empirical model for multispecific antibody-ligand interactions.

L4 ANSWER 21 OF 30 EMBASE COPYRIGHT (c) 2005 Elsevier B.V. All rights reserved on STN

AN 87107246 EMBASE

DN 1987107246

TI Treatment of cancer pain with epidural butyl-amino-benzoate suspension.

AU Shulman M.

CS Illinois Masonic Medical Center, Chicago, IL 60657, United States

SO Regional Anesthesia, (1987) Vol. 12, No. 1, pp. 1-4.

CODEN: RGANDZ

CY United States

DT Journal

FS 037 Drug Literature Index

024 Anesthesiology

016 Cancer

LA English

ED Entered STN: 911211

Last Updated on STN: 911211

DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

L4 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1987:491359 HCAPLUS

DN 107:91359

TI Evaluation of a screening procedure for basic and neutral drugs: n-butyl chloride extraction and megabore capillary gas chromatography

AU Sharp, M. E.

CS Toxicol. Sect., Forensic Lab. Regina, Regina, SK, 6500, Can.

SO Journal - Canadian Society of Forensic Science (1986), 19(2), 83-101

CODEN: JCFSBP; ISSN: 0008-5030

DT Journal

LA English

AB A procedure involving a rapid BuCl extraction is described for the comprehensive screening, in blood, of 164 basic and neutral drugs of forensic significance. Extraction recoveries were determined for a Megabore capillary gas-chromatog. column and a conventional packed column, with N-specific detection recoveries and retention times are tabulated. Detection limits were <200 mg drug/mL blood.

L4 ANSWER 23 OF 30 EMBASE COPYRIGHT (c) 2005 Elsevier B.V. All rights reserved on STN

AN 78206058 EMBASE

DN 1978206058

TI Temperature and pH sensitivity of the partition coefficient as related to the blood-brain barrier to drugs.

AU Kaufman J.J.; Koski W.S.; Benson D.W.

CS Dept. Anesthesiol., Johns Hopkins Univ. Sch. Med., Baltimore, Md. 21205, United States

SO Experimental Eye Research, (1977) Vol. 25, No. suppl., pp. 201-203.

CODEN: EXERA6

CY United Kingdom

DT Journal

FS 037 Drug Literature Index

008 Neurology and Neurosurgery

030 Pharmacology

LA English

AB The true drug distribution (apparent partition coefficient) of a number of CNS-active drugs was measured as a function of pH and temperature. It was found that the distribution coefficients of narcotics and narcotic antagonists are very sensitive to pH in the range of human physiological blood pH's and are strongly temperature dependent. Therefore, body temperature and blood pH of the patient must be considered when assessing blood-brain and blood-CSF exchange of a given drug.

L4 ANSWER 24 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1967:22233 HCAPLUS

DN 66:22233

TI Structure-R(sub f) correlations in the thin-layer chromatography of some basic drugs

AU Fike, Winston W.

CS County Coroner's Office, Cleveland, OH, USA

SO Analytical Chemistry (1966), 38(12), 1697-1702

CODEN: ANCHAM; ISSN: 0003-2700

DT Journal

LA English

AB Rf values for 140 basic drugs in 5 chromatographic systems are discussed. Systems A, B, and C consisted of silica gel plates prepared with 0.1M KOH with the following solvents: A cyclohexane-C₆H₆-diethylamine (75:15:10), B MeOH, and C Me₂CO. Systems D and E consisted of silica gel plates prepared using 0.1M NaHSO₄ with solvents: D MeOH, and E 95% EtOH. A 1% solution of I in MeOH was used as a general locating agent because it gave a pos. test with all the drugs. Several other spray reagents are proposed. Correlations of a more general nature between Rf values in the 5 systems and the presence of particular chemical groups in these compds. are made. It was seen that steric hindrance around the group responsible for the bonding to silica in a particular system, the basicity of the compound, and the presence or absence of a pyridyl ring influenced Rf values to the greatest extent. 18 references.

L4 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1967:16972 HCAPLUS

DN 66:16972

TI Identification of therapeutically significant organic bases by thin-layer chromatography

AU Sunshine, Irving; Fike, Winston W.; Landesman, Halle

CS Sch. of Med., Western Reserve Univ., Cleveland, OH, USA

SO Journal of Forensic Sciences (1966), 11(3), 428-39

CODEN: JFSCAS; ISSN: 0022-1198

DT Journal

LA English

AB Rf data for 138 therapeutically significant organic bases were determined in each of 7 chromatographic systems. If Rf data are determined in only 4 systems, 113 drugs can be characterized. If all 7 systems are used, the remaining 25 drugs can be separated into 19 individual and 3 paired entities. Supports were silica gel G (slurried in 0.1N NaOH or 0.1N KHSO₄) or Chromedia (slurried in 5% NaH₂PO₄). Developing solvents were 95% EtOH, cyclohexane-C₆H₆-Et₂NH (75:15:10 by volume) MeOH, Me₂CO, MeOAc, BuOH-5% citric acid (90:10 by volume). Spray reagents were I₂ in MeOH, Dragendorff reagent, 5% NaNO₂, and K iodoplatinate. Spots were also located by uv absorption.

L4 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1954:5107 HCAPLUS

DN 48:5107

OREF 48:951e-i, 952a-b

TI Determination of alkaloids in organic solution. Action of flavianic acid

AU Wachsmuth, H.
SO Journal de Pharmacie de Belgique (1953), 8, 283-9
CODEN: JPBEAJ; ISSN: 0047-2166
DT Journal
LA Unavailable
AB cf. C.A. 47, 9559d. The addition of flavianic acid in EtOH-Et2O to the base or salt in Et2O or EtOH-Et2O yields the following results: morphine, sensitive 1:700,000, long needles (slowly), in dilute solution turbidity resolving into rosaceous crystals along the sides; codeine, flocculent precipitate of very thin crystals in microscopic rose pattern, sensitive 1:500,000; papaverine, sensitive 1:500,000, yellow precipitate very slowly forming long prisms; heroine, small clumps of very fine needles; dionine, precipitate of clumped fine crystals appearing as amorphous spheres under low magnification; eucodal, large clumps of fine needles; hyoscyamine, whitish precipitate, long slender flexible needles from dilute solution; homatropine, macroscopic needles; sparteine sulfate, large frequently connected needles; hydrastinine, almost immediate formation of long, fine, curved needles; caffeine and theophylline, gradual formation of crystals in double fan or sheaves; theobromine, practically insol. in EtOH and Et2O, no reaction; procaine, clumps; pontocaine, long needles; stovaine, prismatic needles; anesthine, silky needles; scuroform, small quadrangular crystals; orthoform, immediate formation of macroscopic crystals; cycloform, very small whitish sharp needles; pyridine, after 24 hrs. long macroscopic needles; nicotinamide, well-formed crystalline branches; choline, inclined quadratic prisms, sometimes in clumps from very dilute solution; acetylcholine, double sheaves or fans of crystals, very rarely complete spheres; pervitine-HCl, very slow formation of clumps with large branches; eupaverine, difficult crystallization, spearheads; pilocarpine, abundant precipitate, large clumps of fine needles; strychnine, sharp needles; ephedrine, sensitive 1:25,000, small needles; stypticine, clumps of several mm., macroscopic sharp, slight needles; euphylline, small needles; coramine, needles; sulfaguanidine, macroscopic clumps; methenamine, prisms after 24 hrs.; colchicine, small crystals but the precipitate is not always entirely crystalline; benadryl, turbidity slowly resolved to long macroscopic needles; privine, slowly formed small crystals connected at the base; remifon, slow formation of small clumps, slender, curved needles; dramamine, slow formation of long macroscopic needles. Abundant ppts. are obtained with euquinine, nicotine, antipyrine, aconitine, scopolamine, pyramidon (fine needles after several hrs.), dilaudid, emetine, yohimbine, quinidine, sulfadiazine, and cibazol (sensitive 1:1,000,000). Flavianic acid is less active with dicodid, and practically inactive with benzedrine, methionine, vitamin B1, coniine, cardiazol, and hydrastinine. It ppts. methyl orange, methyl red, lysine, tryptophan, and arginine. It ppts. protoporphyrin ethyl ether in CHCl3. Results of quant. precipitation of flavianates of pontocaine, orthoform, homatropine-HBr, sparteine-H2SO4, scuroform, anesthine, pervitine-HCl, brucine, and morphine are given with modifications of the general procedure where necessary.

L4 ANSWER 27 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1947:35442 HCAPLUS

DN 41:35442

OREF 41:7045i,7046h-i,7047a-c

TI Health hazards of the pharmaceutical industry

AU Watrous, R. M.

CS Abbott Labs., North Chicago

SO British Journal of Industrial Medicine (1947), 4, 111-25

CODEN: BJIMAG; ISSN: 0007-1072

DT Journal

LA Unavailable

AB A review with bibliography. Among the hazards discussed are those arising from ipecacuanha, podophyllum, Aspergillus niger (contaminant of penicillin cultures), anhydrous EtOH formula 12-A (containing 5% benzene), benzene, CHCl3, 1,2-dichloroethane, belladonna alkaloids, atropine sulfate, aconitine-HBr, emetine-HCl, pure desiccated scarlet fever toxin, Cl2, POCl3, COCl2, SOCl2, PCl5, chlorosulfonic acid, fuming sulfuric acid, Me2SO4, nitrosomethyl urethan, diazomethane, nitrosomethylurea, MeBr, EtBr, benzyl chloride, 1-methylbutyl bromide, NaCN, KCN, benzyl cyanide, glacial AcOH, Ac2O, mono- and dichloroacetic acids, Na methylate, Na

ethylate, nitrating agents, Zn powder, H₂, di-chloroethyl acetate, aminothiazole, p-acetylaniline, sulfonyl chloride, pentothal-Na, thiourea, CO, As compds. used in the preparation of arsphenamine and its derivs., aniline, dimethylaniline, halocrine (intermediate in the manufacture of quinacrine-2HCl), quinacrine, acriflavine, nicotinic acid, nicotinamide, penicillin powder, procaine, butyn (butacaine sulfate), butesin (butyl aminobenzoate), neoarsphenamine, 2-methyl-1,4-naphthoquinone (synthetic form of vitamin K), chloramine-T, p-(dichlorosulfamyl)benzoic acid (Halazone), Hg, HgCl₂, Hg oxycyanide, diethylstilbestrol, morphine, codeine, white As, tetrachloroethane, ultraviolet light, visible light, infrared light, equine encephalomyelitis virus, mixture of H₂SO₄ and K₂Cr₂O₇ (cleaning solution), glass wool, cloth made of spun glass fiber, cold atmospheric, and fumes of Pb, Cd, and Zn. Sensitization reactions and dermatitis arising from many of the substances listed are described.

L4 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1944:29895 HCAPLUS

DN 38:29895

OREF 38:4384d-g

TI Several alkaloidal iodoargentates

AU Wachsmuth, H.

SO Natuurwetenschappelijk Tijdschrift (Ghent) (1943), 25, 71-81

From: Chem. Zentr. II, 651(1943).

CODEN: NATGAK; ISSN: 0369-3368

DT Journal

LA Unavailable

AB cf. C. A. 37, 5197.3. A solution of AgI in concentrated aqueous KI is a very sensitive reagent for alkaloids. The alkaloid HCl in H₂O gives a precipitate with specific crystal form and sharp m. p., which crystallizes much better than the corresponding Hg, Bi and Sb compds. The compds. fall into 3 groups: 1 mol. alkaloid, 1 mol. AgI and 1 mol. HI (I), 1:2:1 (II) and 1:5:1 (III). No relation was found with the mono- or dibasic character of the alkaloid. The following iodoargentates were prepared (type given): pilocarpine (I), prisms, difficultly soluble in organic solvents except C₅H₅N, m. 169°; choline (I), m. 183.5-4.5°; ephedrine (I), crystals form rhombs, m. 143-5°; codeine forms a type III complex, prisms, and from the aq-Me₂CO₃ mother liquor a type I complex, light-yellow rosettes, m. 176-8°. The only representative of type II is cocaine, prisms forming rosettes, slightly soluble in H₂O and organic solvents, m. 222°. The following belong to type III: alypine, needles; strychnine, 3-sided crystals; sparteine, star groups; pantocaine, prisms, turning yellow in the air. The following were not classified: papaverine, needles; pentamethylenetetrazole, needles, often forming stars; pyramidone, needles; benzocaine, 0.5-cm. needles from 20% HCl; scuroforme needles; cycloform, plates.

L4 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1927:1074 HCAPLUS

DN 21:1074

OREF 21:157d-f

TI New color reaction for procaine and some other local anesthetics and its application to the determination of procaine

AU Rieoel, E. Raymond; Williams, J. F.

SO Journal of the American Chemical Society (1926), 48, 2871-8

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA Unavailable

AB The addition of a few drops of HCl, NaNO₂ and concentrated NH₄OH in the order named develops an intense yellow color with solns. containing procaine, tutocaine, butyn, butesin, propaesin, benzocaine and orthoform; saligenin gives a yellow color with HCl and NaNO₂ and interferes with the above test; adrenaline responds to the test but the color forms slowly, morphine and apomorphine give a red color with HCl and NaNO₂, becoming mahogany-brown with NH₄OH. The reaction has been extended to a quant. method, the conditions to be observed in order to obtain reliable results being the temperature (20°) amts., concentration and order of addition of the reagents. The concentration of the procaine must lie between 10 and 15 mg. in 10-cc. solution. The accuracy is within 10%. Diluting the yellow soln, obtained at the concentration of

maximum color formation permits a detection of color when the amount of procaine is 0.00045 mg. per cc.; with lower concns. the limit of color formation is reached with 0.005 mg. per cc. The possible interference of admixed materials is discussed.

L4 ANSWER 30 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1917:2677 HCAPLUS

DN 11:2677

OREF 11:523i,524a-i

TI Tests for certain narcotic and anesthetic drugs

AU Hankin, E. H.

CS Agra, India

SO India J. Med. Research (1916), 4, 237-55

DT Journal

LA Unavailable

AB Nitric acid test: A small quant. of the substance is placed in a porcelain basin, HNO₃ added from a fine pipet sufficient to wet the substance, the basin heated over a flame, then removed and water added. Cycloform gives a pale yellow color in the cold, which deepens on heating changing to black, forming a black oily liquid. On adding H₂O the oily liquid floats, breaking up into small droplets. This is characteristic for cycloform. Holocain is at first colorless, and after several sec. gives a pale reddish brown color. Orthoform instantly turns black and then rapidly to dark brown. Antipyrine turns yellow and becomes black on heating. If the heat continues long enough the mass deflagrates violently, giving a white smoke with an odor resembling isocyanide. If a slight excess HNO₃ be added the yellow color changes to crimson. The crimson color is obtained immediately if antipyrine is dropped into hot HNO₃. The color reactions for 90 compds. are given in table form. Permanganate film test: See C. A. 5, 2145. Fehling solution: If a small quant. of Fehling solution be added to a solution of anesthesin in 0.5% HCl a white precipitate is produced. After a few min. this precipitate forms large rod-like crystals easily visible to the naked eye. With cocaine, alypin, eucaïn, novocaine, stovaine and tropacocaine, Fehling solution produces a white precipitate, which consists of oily drops. Brucine and strychnine give white crystalline ppts., which do not change on keeping. Granular white ppts. are obtained from acoïne, aconitine, cycloform, holocaine, quinine, quinine-urea and yohimbine. A yellow or greenish yellow precipitate is given by chloretone and brometone. Orthoform yields a yellowish or greenish turbidity; after a short time the liquid becomes transparent and has a sage green color, which darkens after a few hrs., and has a reddish tint. Melting on a glass slide: In certain cases on cooling the substance crystallizes, and the crystalline film thus produced has a characteristic appearance. Cycloform and anesthesin yield films containing minute oval spaces in rows. Tetronal and trional yield films having much larger oval spaces. Oval spaces are sometimes produced by antipyrin but numerous cracks both transverse and longitudinal are also present. Sulfuric acid and potassium iodate: Yohimbine gives a distinctive test when dissolved in a few drops concentrated H₂SO₄ and the KIO₃ added. Zones of bright reddish brown and bluish gray are formed within a few min. Practically identical colors are produced by quebrachin (these may be identical). Morphine, heroine and codeine yield shades of brown or yellowish brown and greenish or blackish gray. Benzoic acid gives a play of colors similar to that given by cocaine. Urotropine test: This test (Pisani, C. A. 9, 511) is not useful for cocaine as the color is not prominent and the same reaction is obtained with eucaïne and tropacocaine. The color reactions of several compds. with urotropine are given. Bromine test: Saporetti (Boll. chim. farm. 1999, 479) first pointed out that Br could be used to distinguish the cocaine derivs. Acoïne gives a white precipitate changing rapidly to pale brown. The white is difficult to see because of the rapid change. Alypin gives a yellow precipitate which dissolves on boiling and reappears on cooling. Anesthesin gives a white precipitate not changed by boiling. If Br enough to color the precipitate has been added the precipitate may dissolve on boiling. Cocaine gives a yellow precipitate soluble on heating. Cycloform gives a white precipitate unchanged by heating. Holocaine gives a yellow precipitate or with more Br a pale yellowish brown precipitate. On heating the precipitate dissolves, if small amts. of Br were used. Nirvanin gives a yellow precipitate, soluble on heating, giving a red solution with a pleasant smell. Novocaine gives a yellow precipitate soluble on heating. If sufficient of the components be

present some reddish oily drops are formed on heating and on cooling a white crystalline precipitate appears. Orthoform, in dilute HCl, gives a dirty green precipitate changing to an orange liquid on heating. Stovaine gives a yellow precipitate easily soluble on heating. Tropacocaine gives a yellow precipitate soluble on heating. The liquid becomes turbid on cooling. Many compds. are classified depending on whether or not they give a precipitate with Br water. The chemical constitution and the melting points are given.